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Sr_3MgPtO_6

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Mg–O) = 0.004 Å
R factor = 0.024
wR factor = 0.049
Data-to-parameter ratio = 24.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Single crystals of the mixed alkaline earth platinate, tristrontium magnesium platinum hexaoxide, Sr_3MgPtO_6, were grown from a KOH flux at 1273 K. The compound adopts the rhombohedral K_4CdCl_6 structure type, featuring chains of face-shared, distorted MgO_6 trigonal prisms (Mg site symmetry 32) and PtO_6 octahedra (Pt site symmetry $\overline{3}$) surrounded by columns of Sr^{2+} ions (Sr site symmetry 2).

Comment

The structure of Sr_3MgPtO_6 was determined in 1997 (Núñez *et al.*, 1997) by powder X-ray diffraction on a polycrystalline sample prepared by conventional sintering techniques, and was shown to adopt the K_4CdCl_6 structure type (Bergerhoff & Schmitz-Dumont, 1956). This structure type features two crystallographically and chemically distinct K^+ positions and consists of chains along [001] of face-shared, distorted KCl_6 trigonal prisms and $CdCl_6$ octahedra. The polyhedral chains are surrounded by spiral columns of K^+ ions. To date, a large and compositionally diverse group of oxides adopting this structure type has been reported, typically as polycrystalline materials [reviewed in Stitzer *et al.* (2001)]. High-temperature flux growth from molten KOH has proven to be an effective oxide crystal growth medium. Single crystals of Sr_3MgPtO_6 were readily grown from molten KOH at 1273 K, using

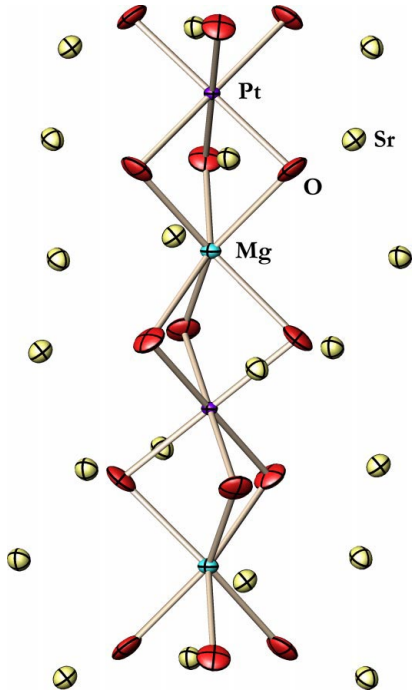

Figure 1
Fragment of the face-shared polyhedral chains in Sr_3MgPtO_6. Displacement ellipsoids are drawn at the 90% probability level.

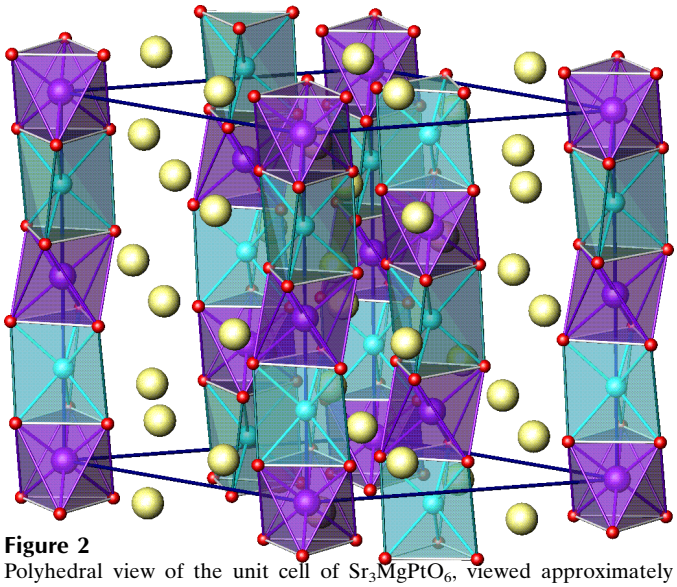

Figure 2
Polyhedral view of the unit cell of Sr_3MgPtO_6, viewed approximately along [110].

$(NH_4)_2PtCl_6$ as the platinum source. Sr_3MgPtO_6 represents an Mg-substituted form of the K_4CdCl_6-type oxide Sr_4PtO_6 (Randall & Katz, 1959), with Mg ordered in the trigonal prism site (site-symmetry 32, Wyckoff symbol 6*a*) and Pt^{4+} in a rhombohedrally elongated octahedral site (site symmetry $\overline{3}$, Wyckoff symbol 6*b*). Fig. 1 illustrates the local coordination of these metal centers. The Sr^{2+} ion resides in an irregular eight-coordinate site (Wyckoff symbol 18*e*) of site symmetry 2. Fig. 2 shows a view of the polyhedral chains and Sr^{2+} columns. Bond lengths and angles from the present single-crystal determination of Sr_3MgPtO_6 are very close to those derived from powder data [Mg—O = 2.172 (16) Å, Pt—O = 2.011 (16) Å and Sr—O = 2.498 (17)–2.742 (17) Å]. Refinement of the site occupancies for Mg and Pt showed no significant deviation from whole occupancy, indicating a stoichiometric compound, and no Sr/Mg mixing on the trigonal prism site.

Experimental

The $(NH_4)_2PtCl_6$ precursor was prepared according to a published method (Kaufman, 1967). Subsequently, $SrCO_3$ (Alfa, 99.95%), $MgCO_3$ (Alfa, 99.8%), and $(NH_4)_2PtCl_6$ (stoichiometric amounts, *ca* 1 g total reagent mass) and KOH (Fisher, reagent grade; ~10 times by mass the total reagent amount) were loaded into a covered alumina crucible. The mixture was heated at 1273 K for 2 h, cooled to 1023 K at a rate of 1 K h^{-1}, at which point the furnace was shut off and allowed to cool to room temperature radiatively. The KOH matrix was dissolved with distilled water, leaving plentiful transparent brown crystals with a rhombohedral habit.

Crystal data

Sr_3MgPtO_6
M_r = 578.26
Trigonal, $R\overline{3}c$
a = 9.6432 (4) Å
c = 11.1112 (6) Å
V = 894.82 (7) Å^3
Z = 6
D_x = 6.439 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1132 reflections
θ = 4.2–36.3°
μ = 50.13 mm^{-1}
T = 293 (2) K
Rhombohedron, brown
0.11 × 0.05 × 0.04 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.073, T_{max} = 0.239
2412 measured reflections
490 independent reflections
431 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 36.3°
$h = -16 \rightarrow 7$
$k = -11 \rightarrow 16$
$l = -18 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.049
S = 1.01
490 reflections
20 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.32 e Å^{-3}
$\Delta\rho_{min}$ = −3.12 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00118 (8)

Table 1
Selected geometric parameters (Å).

Sr—O	2.472 (3)	Mg—O	2.177 (3)
Sr—O^{i}	2.637 (3)	Mg—Pt	2.77780 (15)
Sr—O^{ii}	2.663 (3)	Pt—O	2.031 (3)
Sr—O^{iii}	2.731 (3)		

Symmetry codes: (i) $\frac{1}{3}-x+y, y-\frac{1}{3}, \frac{1}{6}+z$; (ii) $\frac{2}{3}-x+y, \frac{1}{3}-x, \frac{1}{3}+z$; (iii) $\frac{2}{3}+y, \frac{1}{3}-x+y, \frac{1}{3}-z$.

Systematic absences in the dataset confirmed a *c*-glide operation, indicating the space groups $R3c$ and $R\overline{3}c$. Preliminary powder X-ray diffraction showed the compound to be isostructural with K_4CdCl_6 (space group $R\overline{3}c$); therefore, the expected centrosymmetric space group was chosen and confirmed by the structure solution. The largest difference peak and hole were located less than 0.8 Å from the Pt atom.

Data collection: *SMART-NT* (Bruker, 1999); cell refinement: *SAINT-Plus-NT* (Bruker, 1999); data reduction: *SAINT-Plus-NT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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